Semiclassical Singularity Propagation Property for Schrödinger Equations

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Abstract

We consider Schrödinger equations with variable coefficients, and it is supposed to be a long-range type perturbation of the flat Laplacian on $\mathbb{R}^n$. We characterize the wave front set of solutions to Schrödinger equations in terms of the initial state. Then it is shown that the singularity propagates following the classical flow, and it is formulated in a semiclassical setting. Methods analogous to the long-range scattering theory, in particular a modified free propagator, are employed.

1 Introduction

Let H be a Schrödinger operator with variable coefficients:

$$H = -\frac{1}{2}\sum_{j,k=1}^{n} \partial_{x_j} a_{jk}(x)\partial_{x_k} + V(x) \quad \text{on } L^2(\mathbb{R}^n),$$

where $n \geq 1$ is the space dimension. Throughout this paper, we always assume $a_{jk}(x)$ and $V(x)$ are real-valued C^∞-class functions. Moreover, we assume:

Assumption A. For each $x \in \mathbb{R}^n$, $(a_{jk}(x))_{j,k}$ is a positive symmetric matrix. There is $\mu > 0$ such that for any multi-index $\alpha \in \mathbb{Z}_+^n$, there is C_α such that

$$\begin{aligned} \left|\partial_x^\alpha\big(a_{jk}(x) - \delta_{jk}\big)\right| &\leq C_\alpha \langle x\rangle^{-\mu-|\alpha|}, \quad x \in \mathbb{R}^n, \\ \left|\partial_x^\alpha V(x)\right| &\leq C_\alpha \langle x\rangle^{2-\mu-|\alpha|}, \quad x \in \mathbb{R}^n. \end{aligned}$$

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Then it is well-known that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$, and we denote the unique self-adjoint extension by the same symbol H. We let $u(t) = e^{-itH}u_0$ be the solution to the time-dependent Schrödinger equation:

$$i\frac{\partial}{\partial t}u(t) = Hu(t), \quad u(0) = u_0, \quad u_0 \in L^2(\mathbb{R}^n).$$

We study the microlocal singularity of $u(t)$. In particular, we characterize the wave front set of $u(t)$ in the nontrapping region, in terms of u_0. In order to describe our main result, we introduce several notations of the classical flow corresponding to H. Let $k(x,\xi)$ be the classical kinetic energy, and let $p(x,\xi)$ be the full Hamiltonian (modulo lower order terms):

$$k(x,\xi) = \frac{1}{2}\sum_{j,k=1}^{n} a_{jk}(x)\xi_j\xi_k, \quad p(x,\xi) = k(x,\xi) + V(x), \quad x,\xi \in \mathbb{R}^n.$$

Let $\exp tH_p$ denote the Hamilton flow generated by a symbol p, i.e., if $(x(t),\xi(t)) = \exp tH_p(x_0,\xi_0)$, then $(x(t),\xi(t))$ is the solution to the Hamilton equation:

$$\frac{d}{dx}x(t) = \frac{\partial p}{\partial \xi}(x(t),\xi(t)), \quad \frac{d}{dx}\xi(t) = -\frac{\partial p}{\partial x}(x(t),\xi(t)), \quad t \in \mathbb{R}$$

with $x(0) = x_0$, $\xi(0) = \xi_0$.

Definition 1. For $(x_0,\xi_0) \in \mathbb{R}^n \times \mathbb{R}^n$,we denote $(\tilde{y}(t),\tilde{\eta}(t)) = \exp tH_k(x_0,\xi_0)$. (x_0,ξ_0) is called *backward nontrapping* if $|\tilde{y}(t)| \to \infty$ as $t \to -\infty$.

For $a \in C^\infty(\mathbb{R}^{2n})$, we denote the Weyl quantization by $a(x,D_x)$:

$$a(x,D_x)u(x) = (2\pi)^{-n}\int e^{i(x-y)\cdot\xi}a((x+y)/2,\xi)u(y)\,dy\,d\xi,$$

where $u \in \mathcal{S}(\mathbb{R}^n)$ (see, e.g., Hörmander [10]). We recall $(x_0,\xi_0) \notin WF(u)$, the wave front set of u, if and only if there exists $a \in C_0^\infty(\mathbb{R}^{2n})$ such that $a(x_0,\xi_0) \neq 0$ and

$$\big\|a_h(x,D_x)u\big\| = O(h^\infty) \quad \text{as } h \to 0,$$

where $a_h(x,\xi) = a(x,h\xi)$ (see, e.g., Martinez [14], Dimassi, Sjöstand [5]).

Theorem 1.1. *Suppose H satisfies Assumption A, and let $u(t) = e^{-itH}u_0$, $u_0 \in L^2(\mathbb{R}^n)$. Suppose, moreover, (x_0,ξ_0) is backward nontrapping, and let $t_0 > 0$. Then $(x_0,\xi_0) \notin WF(u(t_0))$ if and only if there exists $a \in C_0^\infty(\mathbb{R}^{2n})$ such that $a(x_0,\xi_0) \neq 0$ and*

$$\big\|\big(a_h \circ \exp t_0H_p\big)(x,D_x)u_0\big\| = O(h^\infty) \quad \text{as } h \to 0.$$

The main idea of the proof is very simple. Let $a \in C_0^\infty(\mathbb{R}^{2n})$ such that $a(x_0,\xi_0) \neq 0$ and supported in a small neighborhood of (x_0,ξ_0). We note

$$\bigl\|a_h(x,D_x)u(t_0)\bigr\| = \bigl\|e^{it_0H}a_h(x,D_x)e^{-it_0H}u_0\bigr\|.$$

If we formally apply the semiclassical Egorov theorem, we learn that the principal symbol of $e^{it_0H}a_h(x,D_x)e^{-it_0H}u_0$ is given by $a_h \circ \exp t_0H_p$, and we can obtain an asymptotic expansion of the symbol, where all the terms are supported in $\exp(-t_0H_p)(\operatorname{supp} a)$. If this argument is justified, Theorem 1 follows immediately. However, in order to justify this argument in this framework, we need to find a suitable symbol class, which might be time-dependent. Instead of introducing time-dependent symbol class, we employ a scattering theoretical technique, which is an extension of the method used in [17].

Let $W(t,\xi)$ be a solution to the momentum space Hamilton-Jacobi equation, which is constructed in Section 2. We study

$$\Omega(t) := e^{iW(t,D_x)}e^{-itH}$$

instead of e^{-itH} itself. Let

$$(y(t;x_0,\xi_0),\eta(t;x_0,\xi_0)) = \exp tH_p(x_0,\xi_0).$$

If (x_0,ξ_0) is backward nontrapping, then it is shown in Section 2 that

$$\begin{aligned}
\xi_-(-t_0,x_0,\xi_0) &:= \lim_{\lambda\to+\infty} \lambda^{-1}\eta(-t_0;x_0,\lambda\xi_0),\\
z_-(-t_0;x_0,\xi_0) &:= \lim_{\lambda\to+\infty}\Bigl(y(-t_0;x_0,\lambda\xi_0) - \frac{\partial W}{\partial\xi}(-t_0,\eta(-t_0;x_0,\lambda\xi_0))\Bigr)
\end{aligned}$$

exist. We will see that actually ξ_- and z_- are independent of t_0. We will show:

Theorem 1.2. *Suppose H satisfies Assumption A, and let $u(t)$, (x_0,ξ_0), $t_0>0$ as in Theorem 1. Then $(x_0,\xi_0) \in WF(u(t_0))$ if and only if*

$$(z_-(-t_0;x_0,\xi_0),\xi_-(-t_0;x_0,\xi_0)) \in WF\bigl(e^{iW(-t_0,D_x)}u_0\bigr).$$

Since the symbol of

$$e^{-iW(-t_0,D_x)}\bigl(a_h \circ \exp t_0H_p\bigr)(x,D_x)e^{iW(-t_0,D_x)}$$

is essentially supported in a small neighborhood of (z_-,ξ_-), Theorem 1.1 follows from Theorem 1.2 (see Subsection 3.4 for the detail). Theorem 1.2 is proved using an Egorov theorem for $\Omega(t)a_h(x,D_x)\Omega(t)^{-1}$. We note, at least formally,

$$\begin{aligned}
\frac{d}{dt}\Omega(t) &= i\frac{\partial W}{\partial t}(t,D_x)\Omega(t) - ie^{iW(t,D_x)}He^{-itH}\\
&= -i\Bigl\{e^{iW(t,D_x)}He^{-iW(t,D_x)} - \frac{\partial W}{\partial t}(t,D_x)\Bigr\}\Omega(t)\\
&=: -iL(t)\Omega(t).
\end{aligned}$$

Namely, $\Omega(t)$ is the evolution operator generated by a time-dependent self-adjoint operator $L(t)$. The principal symbol of $L(t)$ is given by

$$p\left(x+\frac{\partial W}{\partial \xi}(t,\xi),\xi\right)-\frac{\partial W}{\partial t}(t,\xi)=p\left(x+\frac{\partial W}{\partial \xi}(t,\xi),\xi\right)-p\left(\frac{\partial W}{\partial \xi}(t,\xi),\xi\right)$$

by virtue of the Hamilton-Jacobi equation. This symbol is $O(\langle\xi\rangle^{1-\mu})$ if $t\neq 0$, and hence the speed of the propagation of singularity for $L(t)$ is 0 (away from $t=0$). However, at $t=0$, $L(0)$ has infinite propagation speed, and we observe a jump of the singularity. This propagation of singularity is described by the flow: $t\mapsto(z_-(t;x_0,\xi_0),\xi_-(t;x_0,\xi_0))$, and we can conclude Theorem 1.2.

Study of microlocal singularity of solutions to Schrödinger equation goes back at least to a work by Boutet de Monvel [2] (see also Lascar [13], Yamazaki [25], Zelditch [26]). Investigation to characterize the wave front set of $u(t)$ in terms of the initial state u_0 for variable coefficients Schrödinger equation was started by a work of Craig, Kappeler and Strauss [4]. They showed that the microlocal regularity of the solution along a nontrapping geodesic follows from rapid decay of the initial state in a conic neighborhood of $-\xi_-=-\lim_{t\to-\infty}\xi(t)$. This property is called the microlocal smoothing property, and it was generalized and refined by Wunsch [23], Nakamura [16] and Ito [11]. Microlocal smoothing property in the analytic category was studied by Robbiano and Zuily [19, 20] and Martinez, Nakamura and Sordoni [15]. Results in this paper may be considered as a refinement of these works, and the microlocal smoothing property (in the C^∞-category) follows immediately from Theorem 1.1. Similar characterization of wave front set for solutions to Schrödinger equation is recently obtained by Hassel and Wunsch [8]. They considered the problem in the framework of *scattering metric*, and the assumptions and the proof are quite different. In a previous paper, Nakamura [17] considered the case of short-range perturbations, i.e., $\mu>1$, and the results in this paper are its generalizations.

On the other hand, the singularity of solutions to perturbed harmonic oscillator Schrödinger equation was studied by Zelditch [26], Yajima [24], Kapitanski, Rodnianski and Yajima [12] and Doi [6, 7]. The idea of these papers, especially those by Doi, is closely related to our proof.

Recently, Strichartz estimates for variable coefficient Schrödinger operator was studied by several authors, e.g., Staffilani and Tataru [22], Robbiano and Zuily [21], Burq, Gérard and Tzvetkov [3], Bouclet and Tzvetkov [1]. Strichartz estimate is another expression of the smoothing property of Schrödinger equations, and there should be implicit relationship with our results. In particular, Bouclet and Tzvetkov used the Isozaki-Kitada modifier to treat long-range perturbations, and it is analogous to our modified free propagator, though the formulation and the construction are completely different.

The paper is organized as follows: In Section 2, we consider the classical motions generated by the kinetic energy and the total Hamiltonian. In particular, we construct a solution to the momentum space Hamilton-Jacobi equation and show the existence of the modified classical wave operator. We prove Theorems 1.2 and then Theorem 1.1 in Section 3.

Throughout this paper, we use the following notation: $S(m,g)$ denotes the Hörmander symbol class (cf. Hörmander [10], Chapter 18). For a compact set $K\subset\mathbb{R}^n$, $S_K(m,g)$ denotes the same symbol class restricted to functions on $K\times\mathbb{R}^n$. For a symbol $a(x,\xi)$, $a(x,D_x)$ denotes the Weyl quantization of a.

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2 Hamilton flows and solution to the Hamilton-Jacobi equation

2.1 Properties of nontrapping geodesic flow

Here we consider the Hamilton flow for the kinetic energy: $k(x,\xi)=\frac{1}{2}\sum a_{jk}(x)\xi_j\xi_k$. We always suppose Assumption A is satisfied.

Proposition 2.1. *Let $(x_0,\xi_0)\in\mathbb{R}^{2n}$ and suppose (x_0,ξ_0) is backward non-trapping. Then there exists $C>0$ such that*

$$|\tilde{y}(t)|\geq C^{-1}|t|-C,\qquad t\leq 0,$$

where

$$(\tilde{y}(t),\tilde{\eta}(t))=(\tilde{y}(t;x_0,\xi_0),\tilde{\eta}(t;x_0,\xi_0))=\exp tH_k(x_0,\xi_0).$$

Moreover, C is taken locally uniformly with respect to (x_0,ξ_0)

Proof. At first we recall the conservation of the energy:

$$k(\tilde{y}(t),\tilde{\eta}(t))=\frac{1}{2}\sum_{j,k}a_{jk}(\tilde{y}(t))\tilde{\eta}_j(t)\tilde{\eta}_k(t)=k(x_0,\xi_0).$$

By the uniform ellipticity of $k(x,\xi)$, we learn that there exists $C_1>0$ such that

$$C_1^{-1}\leq|\tilde{\eta}(t)|\leq C_1,\qquad t\in\mathbb{R}.$$

We compute

$$\begin{aligned}\frac{d^2}{dt^2}|\tilde{y}(t)|^2&=2\frac{d}{dt}\left(\tilde{y}(t)\cdot\frac{d\tilde{y}}{dt}(t)\right)=2\frac{d}{dt}\left(\sum_{j,k}a_{jk}(\tilde{y}(t))\tilde{y}_j(t)\tilde{\eta}_k(t)\right)\\&=4k(\tilde{y}(t),\tilde{\eta}(t))+\tilde{U}(\tilde{y}(t),\tilde{\eta}(t)),\end{aligned}$$

where

$$\tilde{U}(x,\xi) = 2\sum_{j,k,\ell} a_{jk}(x)\big(a_{j\ell}(x)-\delta_{j\ell}\big)\xi_\ell\xi_k$$
$$-\sum_{j,k,\ell,m} a_{jk}(x)\frac{\partial a_{\ell m}}{\partial x_k}(x)x_j\xi_\ell\xi_m + 2\sum_{j,k,\ell,m}\frac{\partial a_{jk}}{\partial x_\ell}(x)a_{\ell m}(x)x_j\xi_k\xi_m.$$

By Assumption A, it is easy to see

$$|\tilde{U}(x,\xi)| \le C\langle x\rangle^{-\mu}|\xi|^2,$$

and this implies

$$\frac{d^2}{dt^2}|\tilde{y}(t)|^2 \ge 4k(x_0,\xi_0) - C\langle\tilde{y}(t)\rangle^{-\mu}|\tilde{\eta}(t)|^2.$$

We can choose $R>0$ so large that

$$4k(x_0,\xi_0) - CR^{-\mu}C_1^2 \ge \varepsilon > 0.$$

Since (x_0,ξ_0) is backward nontrapping, there exists $t_0<0$ such that

$$|\tilde{y}(t_0)| = R, \quad \frac{d}{dt}|\tilde{y}(t_0)| \le 0,$$

and hence

$$\frac{d^2}{dt^2}|\tilde{y}(t_0)|^2 \ge \varepsilon.$$

Then by the convexity of $|\tilde{y}(t)|^2$, we conclude

$$|\tilde{y}(t)|^2 \ge R + \varepsilon(t_0-t)^2/2, \qquad t\le t_0,$$

and the assertion follows immediately. □

Proposition 2.2. *Suppose (x_0,ξ_0) is backward nontrapping. Then*

$$\xi_- := \lim_{t\to-\infty}\tilde{\eta}(t;x_0,\xi_0)$$

exists.

Proof. By Proposition 2.1 and Assumption A, we learn

$$\frac{d}{dt}\tilde{\eta}_j(t) = -\frac{1}{2}\sum_{k,\ell}(\partial_{x_j}a_{k\ell})(\tilde{y}(t))\tilde{\eta}_k(t)\tilde{\eta}_\ell(t)$$
$$= O(|\tilde{y}(t)|^{-1-\mu}) = O(\langle t\rangle^{-1-\mu})$$

as $t\to-\infty$. Hence

$$\xi_- = \lim_{t\to-\infty}\tilde{\eta}(t) = \xi_0 - \int_{-\infty}^0 \frac{d}{dt}\tilde{\eta}(t)dt$$

exists. □

By the above proof, we also observe

$$|\xi_- - \tilde{\eta}(t)| \leq C\langle t\rangle^{-\mu}, \quad t \to -\infty,$$

and C can be taken locally uniformly in (x_0, ξ_0). Let $0 < \delta_1 < 1$, $R > 0$, and we set

$$\Omega_{R,\delta_1} = \left\{(x,\xi) \in \mathbb{R}^{2n} \;\middle|\; R-1 < |x| < R+1, \tfrac{1}{2} < |\xi| < 2, x\cdot\xi \leq -\delta_1|x|\,|\xi|\right\}$$

be a neighborhood of $\left\{(x, -x/|x|) \in \mathbb{R}^{2n} \;\middle|\; |x| = R\right\}$. We fix $\delta_1 > 0$. If R is sufficiently large, we have

$$\begin{aligned}
\frac{d}{dt}|\tilde{y}(t)|^2\Big|_{t=0} &= \sum_{j,k} a_{jk}(x)x_j\xi_k \\
&= x\cdot\xi + \sum_{j,k}(a_{jk}(x) - \delta_{jk})x_j\xi_k \\
&\leq -\delta_1|x|\,|\xi| + \frac{\delta_1}{2}|x|\,|\xi| = -\frac{\delta_1}{2}|x|\,|\xi|
\end{aligned}$$

for $(x,\xi) \in \Omega_{R,\delta_1}$. Hence, in particular, (x,ξ) is backward nontrapping and

$$|\tilde{y}(t)|^2 \geq |x|^2 + \frac{\delta_1}{8}|x|\,|t| + \varepsilon|t|^2 \qquad \text{for } t \leq 0.$$

Thus we have proved the following assertion:

Proposition 2.3. *Let $0 < \delta_1 < 1$. There exist $R_0 > 0$ and $\delta_2 > 0$ such that if $R \geq R_0$ then*

$$|\tilde{y}(t;x,\xi)| \geq |x| + \delta_2|t|, \qquad t \leq 0, \;\; (x,\xi) \in \Omega_{R,\delta_1}.$$

We note that since $k(x,\xi)$ is homogeneous in ξ, the flow also has the following homogeneity: for $\lambda > 0$,

$$\begin{aligned}
\tilde{y}(t;x,\lambda\xi) &= \tilde{y}(\lambda t;x,\xi), \\
\tilde{\eta}(t;x,\lambda\xi) &= \lambda\tilde{\eta}(\lambda t;x,\xi).
\end{aligned}$$

Thus we learn the following property concerning the high energy asymptotics of the geodesic flow:

Proposition 2.4. *(i) Suppose (x_0,ξ_0) is backward nontrapping. Then for any $t < 0$, $\lambda > 0$,*

$$|\tilde{y}(t;x_0,\lambda\xi_0)| \geq C^{-1}\lambda|t| - C,$$

and

$$\xi_-(x_0,\xi_0) = \lim_{\lambda\to+\infty} \lambda^{-1}\tilde{\eta}(t;x_0,\lambda\xi_0)$$

exists. ξ_- *is independent of* $t<0$.
(ii) Let $0<\delta_1<1$. *Then there exist* $R_0>0$ *and* $\delta_2>0$ *such that if* $R\geq R_0$ *then*

$$|\tilde{y}(t;x,\xi)|\geq |x|+\delta_2|t|\,|\xi|$$

for $t\leq 0$ *and*

$$(x,\xi)\in\big\{(x,\xi)\in\mathbb{R}^{2n}\;\big|\;R-1<|x|<R+1, x\cdot\xi\leq-\delta_1|x|\,|\xi|\big\}.$$

In particular,

$$\xi_-(x,\xi)=\lim_{\lambda\to+\infty}\lambda^{-1}\tilde{\eta}(t;x,\lambda\xi),\qquad (x,\xi)\in\Omega_{R,\delta_1},$$

converges uniformly in Ω_{R,δ_1}.

2.2 High energy asymptotics of the Hamilton flow

Now we consider the Hamilton flow:

$$(y(t;x,\xi),\eta(t;x,\xi))=\exp tH_p(x,\xi).$$

We recall $(y(t),\eta(t))$ satisfies the Hamilton equation:

$$\begin{aligned}
\frac{d}{dt}y_j(t)&=\sum_{k=1}^n a_{jk}(y(t))\,\eta_k(t),\\
\frac{d}{dt}\eta_j(t)&=-\frac{1}{2}\sum_{j,k=1}^n\frac{\partial a_{k\ell}}{\partial x_j}(y(t))\,\eta_k(t)\,\eta_\ell(t)-\frac{\partial V}{\partial x_j}(y(t)).
\end{aligned}$$

At first we prepare an a priori estimate:

Proposition 2.5. *Let* $T>0$. *Then there exist* $\alpha,\beta,\gamma>0$ *such that*

$$|y(t;x,\xi)|\leq\alpha|\xi|,\quad |\eta(t;x,\xi)|\leq\beta|\xi|$$

if $|\xi|>1$, $t\in[-T,T]$ *and* $|x|\leq\gamma|\xi|$.

Proof. We note

$$p(x,\xi)=k(x,\xi)+V(x)\leq c_1\langle\xi\rangle^2$$

with some $c_1>0$ if $|x|\leq\gamma|\xi|$. The by the conservation of energy, we learn

$$\begin{aligned}
|\eta(t;x,\xi)|&\leq c_2\sqrt{k(y,\eta)}=c_2\sqrt{p(y,\eta)-V(y)}\\
&\leq c_3(\langle\xi\rangle+\langle y\rangle^{((2-\mu)/2})\leq c_3(\langle\xi\rangle+\langle y\rangle).
\end{aligned}$$

Hence we have

$$\Big|\frac{d}{dt}y(t;x,\xi)\Big|\leq c_3(\langle\xi\rangle+\langle y\rangle).$$

By using the Duhamel formula, we obtain

$$|y(t)| \leq e^{c_3 t}|x| + \int_0^t e^{c_3(t-s)} c_3 \langle \xi \rangle ds \leq c_4 \langle \xi \rangle$$

if $0 \leq t \leq T$ and $|x| \leq \gamma |\xi|$. Then under the same assumption we also have

$$|\eta(t)| \leq c_3(\langle \xi \rangle + \langle y \rangle) \leq c_5 \langle \xi \rangle.$$

The case $-T \leq t \leq 0$ is similar, and we omit the detail. $\square$

If we denote

$$\begin{aligned} y^\lambda(t; x, \xi) &= y(t/\lambda; x, \lambda\xi), \\ \eta^\lambda(t; x, \xi) &= \frac{1}{\lambda}\, \eta(t/\lambda; x, \lambda\xi), \end{aligned}$$

for $\lambda > 0$, then $(y^\lambda(t), \eta^\lambda(t))$ satisfies

$$\begin{aligned} \frac{d}{dt} y_j^\lambda(t) &= \sum_k a_{jk}(y^\lambda)\, \eta_k^\lambda, \\ \frac{d}{dt} \eta_j^\lambda(t) &= -\frac{1}{2} \sum_{k,\ell} \frac{\partial a_{k\ell}}{\partial x_j}(y^\lambda)\, \eta_k^\lambda\, \eta_\ell^\lambda - \frac{1}{\lambda^2} \frac{\partial V}{\partial x_j}(y^\lambda), \end{aligned}$$

with the initial condition: $y^\lambda(0) = x$, $\eta^\lambda(0) = \xi$. By the continuity of the solutions to ODE's in the coefficients, we learn

$$y^\lambda(t) \to \tilde{y}(t), \quad \eta^\lambda(t) \to \tilde{\eta}(t) \quad \text{as } \lambda \to +\infty,$$

locally uniformly in $t \in \mathbb{R}$. In particular, if (x, ξ) is nontrapping, then for any $R > 0$, $|y^\lambda(t)| > R$ for $t \ll 0$ and $\lambda \gg 0$. In fact, we have the following stronger assertion:

Proposition 2.6. *Suppose (x, ξ) is backward nontrapping, and let $t_0 < 0$. Then there exist $C > 0$ and $\lambda_0 > 0$ such that*

$$|y^\lambda(t)| \geq C^{-1}|t| - C, \qquad \text{for} \quad \lambda t_0 \leq t \leq 0,\ \lambda \geq \lambda_0,$$

where $y^\lambda(t) = y^\lambda(t; x, \xi)$. Moreover, C can be taken locally uniformly with respect to (x, ξ).

Proof. The proof is analogous to Proposition 2.1. By Proposition 2.5, we have

$$|y^\lambda(t)| \leq \alpha\, \lambda |\xi| \quad \text{for } \lambda t_0 \leq t \leq 0,$$

if λ is sufficiently large (so that $|x| \leq \beta\, \lambda |\xi|$). As in the proof of Proposition 2.1, we have

$$\frac{d^2}{dt^2} |y^\lambda(t)|^2 = 4 p^\lambda(y^\lambda(t), \eta^\lambda(t)) + U(y^\lambda(t), \eta^\lambda(t)),$$

where

$$p^\lambda(x,\xi) = \frac{1}{2}\sum_{j,k=1}^{n} a_{jk}(x)\,\xi_j\,\xi_k + \frac{1}{\lambda^2}V(x),$$
$$U(x,\xi) = \tilde{U}(x,\xi) - \frac{4}{\lambda^2}V(x) - \frac{2}{\lambda^2}\sum_{j,k} a_{jk}(x)\,x_j\,\frac{\partial V}{\partial x_k}(x).$$

These imply

$$\frac{d^2}{dt^2}|y^\lambda(t)|^2 \geq 4k(x,\xi) - C\lambda^{-\mu} - C\langle y^\lambda(t)\rangle^{-\mu}.$$

Then, by noting the above remark that $y^\lambda(t) \to \tilde{y}(t)$ as $\lambda \to +\infty$, the same argument as in the proof of Proposition 2.1 applies, and we conclude the assertion. □

Corollary 2.7. *Let (x,ξ), t_0, C and λ_0 as in Proposition 2.6. Then*

$$|y(t;x,\lambda\xi)| \geq C^{-1}\,\lambda|t| - C \quad \text{for } t_0 \leq t \leq 0,\ \lambda \geq \lambda_0.$$

As well as Proposition 2.4, we also have the following proposition:

Proposition 2.8. *Let $0 < \delta_1 < 1$ and $t_0 < 0$. Then there exist $R_0 > 0$, $\delta_2 > 0$ and $\lambda_0 > 0$ such that if $R \geq R_0$ then*

$$|y(t;x,\xi)| \geq |x| + \delta_2\,|t|\,|\xi|, \qquad t_0 \leq t \leq 0,$$

for $(x,\xi) \in \big\{(x,\xi)\ \big|\ R-1 < |x| < R+1, |\xi| \geq \lambda_0, x\cdot\xi \leq -\delta_1|x|\,|\xi|\big\}$.

Proposition 2.9. *Suppose (x,ξ) is backward nontrapping. Then for any $t_0 < 0$, there exists $C > 0$ such that*

$$|\eta(t;x,\lambda\xi) - \tilde{\eta}(t;x,\lambda\xi)| \leq C\lambda^{1-\mu}|t|^{2-\mu},$$
$$|y(t;x,\lambda\xi) - \tilde{y}(t;x,\lambda\xi)| \leq C\lambda^{1-\mu}|t|^{3-\mu}$$

for $t \in [t_0, -1/\lambda]$ and $\lambda > 1$.

Proof. It suffices to show the equivalent assertion:

$$|\eta^\lambda(t;x,\xi) - \tilde{\eta}(t;x,\xi)| \leq C\lambda^{-2}|t|^{2-\mu},$$
$$|y^\lambda(t;x,\xi) - \tilde{y}(t;x,\xi)| \leq C\lambda^{-2}|t|^{3-\mu}$$

for $t \in [\lambda t_0, -1]$. By the Hamilton equation, we have

$$\frac{d}{dt}\Big(\eta_j^\lambda(t) - \tilde{\eta}_j\Big) = -\frac{1}{2}\sum_{k,\ell}\bigg(\frac{\partial a_{k\ell}}{\partial x_j}(y^\lambda)\,\eta_k^\lambda\,\eta_\ell^\lambda - \frac{\partial a_{k\ell}}{\partial x_j}(\tilde{y})\,\tilde{\eta}_k\,\tilde{\eta}_\ell\bigg) - \frac{1}{\lambda^2}\frac{\partial V}{\partial x_j}(y^\lambda),$$
$$\frac{d}{dt}\Big(y_j^\lambda(t) - \tilde{y}_j(t)\Big) = \sum_k\Big(a_{jk}(y^\lambda)\,\eta_k^\lambda - a_{jk}(\tilde{y})\,\tilde{\eta}_k\Big).$$

These imply

$$\left|\frac{d}{dt}\Big(\eta^\lambda-\tilde\eta\Big)\right| \le c_1\Big(|t|^{-1-\mu}|\eta^\lambda-\tilde\eta|+|t|^{-2-\mu}|y^\lambda-\tilde y|+\lambda^{-2}|t|^{1-\mu}\Big),$$
$$\left|\frac{d}{dt}\Big(y^\lambda-\tilde y\Big)\right| \le c_1|\eta^\lambda-\tilde\eta|+c_1|t|^{-1-\mu}|y^\lambda-\tilde y|,$$

for $t\le -1$ with some $c_1>0$ (cf. Lemma A.1 in Appendix). If $t\le -T<0$, we have

$$\left|\frac{d}{dt}\Big(\eta^\lambda-\tilde\eta\Big)\right| \le c_1\Big(T^{-\mu}|t|^{-1}|\eta^\lambda-\tilde\eta|+T^{-\mu}|t|^{-2}|y^\lambda-\tilde y|+\lambda^{-2}|t|^{1-\mu}\Big),$$
$$\left|\frac{d}{dt}\Big(y^\lambda-\tilde y\Big)\right| \le c_1|\eta^\lambda-\tilde\eta|+c_1T^{-\mu}|t|^{-1}|y^\lambda-\tilde y|.$$

Thus, for $t<-T$, $|\eta^\lambda-\tilde\eta|$ and $|y^\lambda-\tilde y|$ are majorized by a solution to

$$-Z'\ge c_1\Big(T^{-\mu}|t|^{-1}Z+T^{-\mu}|t|^{-2}Y+\lambda^{-2}|t|^{1-\mu}\Big),$$
$$-Y'\ge Z+c_1T^{-\mu}|t|^{-1}Y$$

with

$$Z(-T)\ge|\eta^\lambda(-T)-\tilde\eta(-T)|,\quad Y(-T)\ge|y^\lambda(-T)-\tilde y(-T)|.$$

If we set

$$Y(t)=c_2\lambda^{-2}|t|^{3-\mu},\quad Z(t)=c_3\lambda^{-2}|t|^{2-\mu},$$

then the differential inequalities are satisfied if

$$c_3(2-\mu)\ge c_1\big(c_3T^{-\mu}+c_2T^{-\mu}+1\big);$$
$$c_2(3-\mu)\ge c_1c_3+c_1c_2T^{-\mu}.$$

In other words, if

$$c_3((2-\mu)-c_1T^{-\mu})\ge c_1c_2T^{-\mu}+c_1;$$
$$c_2((3-\mu)-c_1T^{-\mu})\ge c_1c_3.$$

We choose T so large that

$$((2-\mu)-c_1T^{-\mu})^{-1}\times c_1^2T^{-\mu}((3-\mu)-c_1T^{-\mu})^{-1}<1,$$

and set $c_3=((3-\mu)-c_1T^{-\mu})c_1^{-1}c_2$. If c_2 is sufficiently large, the above inequalities are satisfied.

Since $|y^\lambda(-T)-\tilde y(-T)|$, $|\eta^\lambda(-T)-\tilde\eta(-T)|=O(\lambda^{-2})$ as $\lambda\to+\infty$, the initial condition is also satisfied if c_2 is taken sufficiently large. Thus we conclude the assertion for $t\in[\lambda t_0,-T]$. The estimate for $t\in[-T,-1]$ is obvious. □

Proposition 2.9 implies, in particular,

$$\lim_{\lambda\to+\infty}\lambda^{-1}\eta(t;x,\lambda\xi)=\lim_{\lambda\to+\infty}\lambda^{-1}\tilde\eta(t;x,\lambda\xi)=\xi_-(x,\xi).$$

2.3 Construction of a solution to the Hamilton-Jacobi equation

In order to construct a solution to the momentum space Hamilton-Jacobi equation, we prepare one more lemma about the classical flow:

Proposition 2.10. *Let $\delta_1 > 0$ and $t_0 < 0$. There exist $R_0 > 0$, $c_0 > 0$ and $C > 0$ such that*

$$\left|\frac{\partial}{\partial x}\eta(t;x,\xi)\right| \le CR^{-1-\mu}|\xi|,$$
$$\left|\frac{\partial}{\partial \xi}(\eta(t;x,\xi)-\xi)\right| \le CR^{-\mu}$$

for $t_0 \le t \le 0$,

$$(x,\xi) \in \Omega := \left\{(x,\xi)\in\mathbb{R}^{2n} \;\middle|\; \big||x|-R\big| \le 1, |\xi| \ge \lambda, x\cdot\xi \le -\delta_1|x|\cdot|\xi|\right\}$$

with $R \ge R_0$ and $\lambda \ge c_0 R$. Moreover, for any $\alpha,\beta \in \mathbb{Z}_+^n$, there is $C_{\alpha\beta} > 0$ such that

$$\left|\left(\frac{\partial}{\partial x}\right)^\alpha\left(\frac{\partial}{\partial \xi}\right)^\beta(y(t;x,\xi)-x)\right| \le C_{\alpha\beta}\,|t|\,\langle\xi\rangle^{1-|\beta|},$$
$$\left|\left(\frac{\partial}{\partial x}\right)^\alpha\left(\frac{\partial}{\partial \xi}\right)^\beta(\eta(t;x,\xi)-\xi)\right| \le C_{\alpha\beta}\,\langle\xi\rangle^{1-|\beta|},$$

for $(x,\xi)\in\Omega$ and $t\in[t_0,0]$.

Proof. We set $\lambda = |\xi|$ and consider

$$y^\lambda(t;x,\xi) = y(t/\lambda;x,\lambda\xi),$$
$$\eta^\lambda(t;x,\xi) = \lambda^{-1}\eta(t/\lambda;x,\lambda\xi).$$

Then it suffices to show the above estimates for η^λ and y^λ with $|\xi| = 1$, $\lambda \ge \lambda_0$ and $t \in [\lambda t_0, 0]$.

We mimic the argument of Hörmander [9] Lemma 3.7. Let s be a variable x_j or ξ_j, $j = 1,\dots,n$. By the Hamilton equation, we have

$$\frac{d}{dt}\left(\frac{\partial y_j^\lambda}{\partial s}\right) = \sum_{k,\ell}\frac{\partial a_{jk}}{\partial x_\ell}(y^\lambda)\frac{\partial y_\ell^\lambda}{\partial s}\,\eta_k^\lambda + \sum_k a_{jk}(y^\lambda)\frac{\partial \eta_k^\lambda}{\partial s}, \tag{2.1}$$

$$\begin{aligned}\frac{d}{dt}\left(\frac{\partial \eta_j^\lambda}{\partial s}\right) &= -\frac{1}{2}\sum_{k,\ell,m}\frac{\partial^2 a_{k\ell}}{\partial x_j\partial x_m}(y^\lambda)\,\eta_k^\lambda\,\eta_\ell^\lambda\,\frac{\partial y_m^\lambda}{\partial s}\\ &\quad -\sum_{k,\ell}\frac{\partial a_{k\ell}}{\partial x_j}(y^\lambda)\,\eta_k^\lambda\,\frac{\partial \eta_\ell^\lambda}{\partial s} - \frac{1}{\lambda^2}\sum_k\frac{\partial^2 V}{\partial x_k\partial x_j}(y^\lambda)\frac{\partial y_k^\lambda}{\partial s}.\end{aligned} \tag{2.2}$$

Then $|\partial y^\lambda/\partial s|$ and $|\partial\eta^\lambda/\partial s|$ are majorized by a solution to

$$-\frac{d}{dt}Y \geq c_1(R+\delta|t|)^{-1-\mu}Y + c_1 Z,$$
$$-\frac{d}{dt}Z \geq c_1(R+\delta|t|)^{-2-\mu}Y + c_1(R+\delta|t|)^{-1-\mu}Z + \frac{c_1}{\lambda^2}(R+\delta|t|)^{-\mu}Y,$$

with $Y(0)\geq 0$ and $Z(0)\geq 1$ if $s=\xi_j$, $Y(0)\geq 1$ and $Z(0)\geq 0$ if $s=x_j$. Note we consider the inequality in $t<0$.

We set

$$Y = c_2(R-\delta t), \quad Z = c_3(1-(R-\delta t)^{-\mu'}), \quad \lambda t_0 \leq t \leq 0$$

with $0<\mu'<\mu$. Then the differential inequalities for the majorants are satisfied if

$$c_2\delta \geq c_1c_2R^{-\mu} + c_1c_3, \tag{2.3}$$

$$c_3\delta\mu' \geq R^{-(\mu-\mu')}\left(c_1c_2 + c_1c_3 + c_1c_2\left(\frac{R-\delta\lambda t_0}{\lambda}\right)^2\right), \tag{2.4}$$

and $R^{-\mu'}\leq 1/2$ so that $Z>0$. We note

$$\left|\frac{R-\delta\lambda t_0}{\lambda}\right| = \left|\frac{R}{\lambda} - \delta t_0\right| \leq c_0^{-1} + \delta|t_0|$$

since $\lambda > c_0R$. Now we choose $c_2/c_3 = \gamma > 2c_1/\delta$, and choose R_0 so that

$$R_0 > \max\left\{2^{1/\mu'}, \left(\frac{2c_1}{\delta}\right)^{1/\mu}, \left(\frac{\gamma c_1 c_2}{\delta\mu'}\left[1+\gamma^{-1}+(c_0^{-1}+\delta|t_0|)^2\right]\right)^{1/(\mu-\mu')}\right\},$$

then the above conditions are satisfied. Thus we learn

$$\left|\frac{\partial y_j^\lambda}{\partial s}(t)\right| \leq c_2(R-\delta t), \qquad \left|\frac{\partial \eta_j^\lambda}{\partial s}(t)\right| \leq c_2/\gamma,$$

for $R\geq R_0$, $\lambda\geq c_0R$ and $t\in[\lambda t_0, 0]$, provided

$$\left|\frac{\partial y_j^\lambda}{\partial s}(0)\right| \leq c_2R, \qquad \left|\frac{\partial \eta_j^\lambda}{\partial s}(0)\right| \leq c_2/(2\gamma).$$

We now consider the case $s=x_k$. Then we may set $c_2=R^{-1}$ and we have

$$\left|\frac{\partial y_j^\lambda}{\partial x_k}(t)\right| \leq 1 - \frac{\delta t}{R}, \qquad \left|\frac{\partial \eta_j^\lambda}{\partial x_k}(t)\right| \leq \frac{1}{\gamma R}.$$

We integrate the equation (2.2) again to obtain

$$
\begin{aligned}
\left|\frac{\partial \eta_j^\lambda}{\partial x_k}(t)\right| &\le \frac{c_1}{R}\int_t^0 (R-\delta r)^{-1-\mu}dr + \frac{c_1}{\gamma R}\int_t^0 (R-\delta r)^{-1-\mu}dr \\
&\quad + \frac{c_1}{R\lambda^2}\int_t^0 (R-\delta r)^{1-\mu}dr \\
&\le (\left(\frac{c_1}{\mu}+\frac{c_1}{\gamma\mu}\right)R^{-1-\mu} + c_1\left(\frac{R-\delta t}{\lambda}\right)^2 R^{-1-\mu} \\
&\le CR^{-1-\mu}
\end{aligned}
$$

if $t\in[\lambda t_0,0]$ and $\lambda \ge c_0 R$. Similarly, if $s=\xi_k$, we may set $c_2=2\gamma$ and we have

$$
\left|\frac{\partial y_j^\lambda}{\partial \xi_k}(t)\right| \le 2\gamma(R-\delta t), \qquad \left|\frac{\partial \eta_j^\lambda}{\partial \xi_k}(t)\right| \le 2.
$$

By integrating the equation (2.2), we conclude

$$
\left|\frac{\partial \eta_j^\lambda}{\partial \xi_k}(t) - \delta_{jk}\right| \le C' R^{-\mu}.
$$

For higher derivatives, we prove the estimates by induction. It suffices to show

$$
\begin{aligned}
\left|\partial_x^\alpha \partial_\xi^\beta (y^\lambda(t;x,\xi)-x)\right| &\le C_{\alpha\beta}|t|, \\
\left|\partial_x^\alpha \partial_\xi^\beta (\eta^\lambda(t;x,\xi)-\xi)\right| &\le C_{\alpha\beta}
\end{aligned}
$$

for $t\in[\lambda t_0,0]$. We suppose these hold for $|\alpha+\beta|<k$, and let

$$
Y(t)=\partial_x^\alpha\partial_\xi^\beta(y^\lambda(t;x,\xi)-x), \quad Z(t)=\partial_x^\alpha\partial_\xi^\beta(\eta^\lambda(t;x,\xi)-\xi)
$$

with $|\alpha+\beta|=k$. Then by the induction hypothesis, we can show Y and Z satisfy

$$
\begin{aligned}
&Y' = A_{11}Y + A_{12}Z + A_{13}, \\
&Z' = A_{21}Y + A_{22}Z + A_{23} + \lambda^{-2}(A_{31}Y + A_{33}), \\
&Y(0)=Z(0)=0,
\end{aligned}
$$

where

$$
\begin{aligned}
&A_{11}=O(\langle t\rangle^{-1-\mu}), \quad A_{12}=O(1), \quad A_{13}=O(\langle t\rangle^{-\mu}), \\
&A_{21}=O(\langle t\rangle^{-2-\mu}), \quad A_{22}=O(\langle t\rangle^{-1-\mu}), \quad A_{23}=O(\langle t\rangle^{-1-\mu}), \\
&A_{31}=O(\langle t\rangle^{-\mu}), \quad A_{32}=O(\langle t\rangle^{1-\mu}),
\end{aligned}
$$

which itself is proved by induction. Then for $t\in[\lambda t_0,-1]$, we have

$$
\begin{aligned}
&\left|Y'\right| \le c_1(\langle t\rangle^{-1-\mu}|Y| + |Z| + \langle t\rangle^{-\mu}), \\
&\left|Z'\right| \le c_1(\langle t\rangle^{-2-\mu}|Y| + \langle t\rangle^{-1-\mu}|Z| + \langle t\rangle^{-1-\mu}).
\end{aligned}
$$

These imply Y and Z are majorized by $M\langle t\rangle$ and M, respectively, with sufficiently large M (the proof is analogous to the above argument). By integrating the differential equation again, we conclude the assertion for $|\alpha+\beta|=k$. $\square$

We note the above proof for the derivatives works for $(\tilde{y}(t;x,\xi),\tilde{\eta}(t,x,\xi))$ $(t<0)$ if (x,ξ) is backward nontrapping. In particular, we learn that $\partial_t\partial_x^\alpha\partial_\xi^\beta\tilde{\eta}(t;x,\xi)$ is integrable with respect to t in $(-\infty,0]$, and hence we conclude $\partial_x^\alpha\partial_\xi^\beta\tilde{\eta}(t;x,\xi)$ converges as $t\to-\infty$, and the estimate is locally uniform. Thus we have

Corollary 2.11. *Suppose (x,ξ) is backward nontrapping. Then*

$$(x,\xi)\mapsto\xi_-(x,\xi)$$

is a C^∞ map, and $\tilde{\eta}(t;x,\xi)$ converges to $\xi_-(x,\xi)$ locally uniformly with all the derivatives as $t\to-\infty$.

Now we consider the map:

$$\Lambda:\xi\ \longmapsto\ \eta(t;-R\xi/|\xi|,\xi).$$

Proposition 2.10 implies $\left\|\frac{\partial\Lambda}{\partial\xi}-I\right\|=O(R^{-\mu})$ uniformly for $|\xi|\geq c_0R$. We choose R so large that $\frac{\partial\Lambda}{\partial\xi}$ is invertible for $|\xi|\geq c_0R$. It is also easy to see that $|\Lambda-\xi|=O(R^{-\mu}|\xi|)$ for $|\xi|\geq c_0R$, and hence $\mathrm{Ran}\Lambda\supset\{\xi\in\mathbb{R}^n\ \big|\ |\xi|\geq c_4R\}$ with some $c_4>0$. Then we set

$$\zeta(t,\cdot)=\Lambda(t,\cdot)^{-1}\ :\ \{\xi\ \big|\ |\xi|\geq c_4R\}\longrightarrow\mathbb{R}^n,$$

i.e.,

$$\eta(t;-R\zeta(t,\xi)/|\zeta(t,\xi)|,\zeta(t,\xi))=\xi\qquad\text{for } |\xi|\geq c_4R.$$

By Proposition 2.10, we learn

$$\left|\left(\frac{\partial}{\partial\xi}\right)^\alpha\zeta(t,\xi)\right|\leq C_\alpha\langle\xi\rangle^{1-|\alpha|},\qquad t\in[t_0,0],\ |\xi|\geq c_4R. \tag{2.5}$$

Then we set

$$W_1(t,\xi)=\int_0^t\big(p(y(s),\eta(s))+y(s)\cdot\partial_t\eta(s)\big)ds-R|\xi|,\qquad |\xi|\geq c_4R,$$

where

$$y(s)=y(s;-R\zeta(t,\xi)/|\zeta(t,\xi)|,\zeta(t;\xi)),\quad \eta(s)=\eta(s;-R\zeta(t,\xi)/|\zeta(t,\xi)|,\zeta(t;\xi)).$$

It is well-known that $W_1(t,\xi)$ satisfies the Hamilton-Jacobi equation (cf. Reed-Simon [18] Section XI.9):

$$\frac{\partial}{\partial t}W_1(t,\xi)=p\left(\frac{\partial W_1}{\partial\xi}(t,\xi),\xi\right),\qquad |\xi|\geq c_4R.$$

By the construction we have

$$\partial_\xi W_1(t,\xi) = y(t; -R\zeta(t,\xi)/|\zeta(t,\xi)|, \zeta(t;\xi)),$$

and

$$\left|\partial_\xi^\alpha W_1(t,\xi)\right| \le C_\alpha \langle\xi\rangle^{2-|\alpha|}, \qquad t\in[t_0,0],\ |\xi|\ge c_4 R. \tag{2.6}$$

We use a partition of unity to construct $W(t,\xi)$ so that

$$W(t,\xi) = \begin{cases} W_1(t,\xi), & |\xi|\ge c_4R+1, \\ -R|\xi| + t|\xi|^2/2, & |\xi|\le c_4 R. \end{cases}$$

Clearly W satisfies (2.6) as well.

2.4 Modified free motion and asymptotic trajectories

Proposition 2.12. *Suppose (x_0,ξ_0) is backward nontrapping, and let $t_0<0$. Then there exists a neighborhood U of (x_0,ξ_0) in $\mathbb{R}^{2n}$ such that*

$$\begin{aligned} \xi_-(x,\xi) &= \lim_{\lambda\to+\infty} \lambda^{-1}\eta(t_0;x,\lambda\xi), \\ z_-(x,\xi) &= \lim_{\lambda\to+\infty} \left\{ y(t_0;x,\lambda\xi) - \partial_\xi W(t_0,\eta(t_0;x,\lambda\xi)) \right\} \end{aligned}$$

exist for $(x,\xi)\in U$. $\xi_-(x,\xi)$ and $z_-(x,\xi)$ are independent of $t_0<0$. Moreover, the convergence is uniform in U with its derivatives, and

$$S_-:\ (x,\xi)\mapsto(z_-,\xi_-)$$

is a local diffeomorphism.

Remark 2.13. We have already seen ξ_- depends only on $(a_{jk}(x))$, and is independent of $V(x)$. As we will see in the proof, z_- is also independent of $V(x)$, though $W(t,\xi)$ does depend on $V(x)$.

Proof. The convergence of ξ_- is already shown in Proposition 2.9 and its remark. At first, we show

$$z^\lambda(t;x,\xi) = y^\lambda(t;x,\xi) - \partial_\xi W^\lambda(t;\eta^\lambda(t;x,\xi))$$

converges as $\lambda\to\infty$, where $W^\lambda(t,\xi)=W(t/\lambda,\lambda\xi)$ and $t=\lambda t_0$.

For (x,ξ) near (x_0,ξ_0), we choose $\zeta^\lambda\in\mathbb{R}^n$ such that

$$\eta^\lambda(t;x,\xi) = \eta^\lambda(t;-R\zeta^\lambda/|\zeta^\lambda|,\zeta^\lambda),$$

and we set

$$v^\lambda(s) = y^\lambda(s;-R\zeta^\lambda/|\zeta^\lambda|,\zeta^\lambda), \quad w^\lambda(s) = \eta^\lambda(s;-R\zeta^\lambda/|\zeta^\lambda|,\zeta^\lambda)$$

for $s \in [t, 0]$. Note that ζ^λ is a function of x, ξ and $t = \lambda t_0$, and $\partial_x \partial_\xi \zeta^\lambda$ is uniformly bounded by virtue of Proposition 2.10 and discussion after it. We also set

$$a(s) = y^\lambda(s; x, \xi) - v^\lambda(s),$$
$$b(s) = \eta^\lambda(s; x, \xi) - w^\lambda(s).$$

We note

$$|a(0)| = \big|x + R\zeta/|\zeta|\big| \le |x| + R, \quad b(t) = 0.$$

a and b satisfy differential equations:

$$\frac{d}{ds}a(s) = \frac{\partial p^\lambda}{\partial \xi}(y^\lambda, \eta^\lambda) - \frac{\partial p^\lambda}{\partial \xi}(v^\lambda, w^\lambda),$$
$$\frac{d}{ds}b(s) = -\Big(\frac{\partial p^\lambda}{\partial x}(y^\lambda, \eta^\lambda) - \frac{\partial p^\lambda}{\partial x}(v^\lambda, w^\lambda)\Big),$$

where $p^\lambda(x, \xi) = \frac{1}{2}\sum_{j,k} a_{jk}(x)\xi_j\xi_k + \lambda^{-2}V(x)$. Since $\lambda \ge |s/t_0|$, these imply

$$|a'(s)| \le c_1\langle s\rangle^{-1-\mu}|a(s)| + c_1|b(s)|, \tag{2.7}$$
$$|b'(s)| \le c_1\langle s\rangle^{-2-\mu}|a(s)| + c_1\langle s\rangle^{-1-\mu}|b(s)| \tag{2.8}$$

for $s \in [t, 0]$ with some $c_1 > 0$. We note $a(s) = O(\langle s\rangle)$ and $b(s) = O(1)$ by Proposition 2.5. Hence by (2.8), we have

$$|b(s)| = \left|\int_t^s b'(u)du\right| \le c_2\langle s\rangle^{-\mu} = O(\langle s\rangle^{-\mu}).$$

Then we substitute this to (2.7) to obtain

$$|a(s)| = \left|a(0) - \int_s^0 a'(u)du\right| \le |x| + R + c_3\langle s\rangle^{1-\mu} = O(\langle s\rangle^{1-\mu}).$$

Repeating these, we have $|b(s)| = O(\langle s\rangle^{-2\mu})$ and then $|a(s)| = O(\langle s\rangle^{1-2\mu})$ provided $2\mu \le 1$. Iterating this procedure, we arrive at $|a(s)| \le C$ and $|b(s)| \le C\langle s\rangle^{-1-\mu}$. Moreover, we also have

$$|a'(s)| \le c_4\langle s\rangle^{-1-\mu}.$$

We recall that $y^\lambda(s; x, \xi) \to \tilde{y}(s; x, \xi)$ as $\lambda \to \infty$ for each s, and $\eta(t; x, \xi)$ converges to $\xi_-(x, \xi)$ as $\lambda \to \infty$ since $t = \lambda t_0$ with $t_0 < 0$. By the uniform continuity of the inverse of $\Lambda(t, \cdot)$, ζ^λ converges to $\tilde{\zeta}$ as $\lambda \to \infty$, where $\tilde{\zeta}$ is given by $\xi_-(x, \xi) = \xi_-(-R\tilde{\zeta}/|\tilde{\zeta}|, \tilde{\zeta})$. Hence, in particular, $v^\lambda(s)$ converges to $\tilde{y}(s; -R\tilde{\zeta}/|\tilde{\zeta}|, \tilde{\zeta})$ for each s. Then by the dominated convergence theorem,

we learn

$$\lim_{\lambda\to\infty}\big\{y(t_0;x,\lambda\xi)-\partial_\xi W(t_0,\eta(t_0;x,\lambda\xi))\big\}=\lim_{\lambda\to\infty}\big\{y^\lambda(t;x,\xi)-v^\lambda(s)\big\}$$
$$=\lim_{\lambda\to\infty}\left[x+R\,\frac{\zeta^\lambda}{|\zeta^\lambda|}-\int_t^0\frac{d}{ds}(y^\lambda(s;x,\xi)-v^\lambda(s))ds\right]$$
$$=x+R\,\frac{\tilde\zeta}{|\tilde\zeta|}-\int_{-\infty}^0\frac{d}{ds}(\tilde y(s;x,\xi)-\tilde y(s;-R\tilde\zeta/|\tilde\zeta|,\tilde\zeta))ds.$$

Note the right hand side is independent of the potential $V(x)$.

Next we consider the convergence of the derivatives. As in the proof of Proposition 2.10, for any $\alpha,\beta\in\mathbb{Z}_+^n$, we have

$$|\partial_s\,\partial_x^\alpha\partial_\xi^\beta\eta^\lambda(s;x,\xi)|\le C\langle s\rangle^{-1-\mu},\quad \lambda t_0\le s\le 0.$$

Hence, by the dominated convergence theorem, we have

$$\begin{aligned}\lambda^{-1}\partial_x^\alpha\partial_\xi^\beta\eta(t_0;x,\lambda\xi)&=\partial_x^\alpha\partial_\xi^\beta\eta^\lambda(\lambda t_0;x,\xi)\\&=\xi-\int_{\lambda t_0}^0\partial_s\,\partial_x^\alpha\partial_\xi^\beta\eta^\lambda(s;x,\xi)ds\\&\longrightarrow\ \xi-\int_{-\infty}^0\partial_s\partial_x^\alpha\partial_\xi^\beta\tilde\eta(s;x,\xi)ds=\partial_x^\alpha\partial_\xi^\beta\xi_-(x,\xi)\end{aligned}$$

as $\lambda\to\infty$ (cf. Corollary 2.11).

For $z(t;x,\xi)$, we prove the convergence by induction. Let $a(s)$ and $b(s)$ as above, and consider $\partial_x^\alpha\partial_\xi^\beta a(s)$ and $\partial_x^\alpha\partial_\xi^\beta b(s)$. We suppose

$$\big|\partial_x^\alpha\partial_\xi^\beta a(s)\big|\le C,\quad \big|\partial_x^\alpha\partial_\xi^\beta b(s)\big|\le C\langle s\rangle^{-1-\mu},\quad s\in[-\lambda t_0,0]$$

for $|\alpha+\beta|<k$ as our induction hypothesis. Let $|\alpha+\beta|=k$, and set $A(s)=\partial_x^\alpha\partial_\xi^\beta a(s)$ and $B(s)=\partial_x^\alpha\partial_\xi^\beta b(s)$. Then by inductive computations (from the differential equation for $a(s)$ and $b(s)$), we can show (as in the proof of Proposition 2.10), $A(s)$ and $B(s)$ satisfy

$$\begin{aligned}&|A'(s)|\le c_1\langle s\rangle^{-1-\mu}|A(s)|+c_1|B(s)|+c_1\langle s\rangle^{-1-\mu},\\&|B'(s)|\le c_1\langle s\rangle^{-2-\mu}|A(s)|+c_1\langle s\rangle^{-1-\mu}|B(s)|+c_1\langle s\rangle^{-2-\mu}\end{aligned}$$

for $s\in[\lambda t_0,0]$. Note we use a priori estimates: $A(s)=O(\langle s\rangle)$, $B(s)=O(1)$, which follow from Proposition 2.10. Since $A(0)$ is bounded and $B(\lambda t_0)=0$, we can use the same argument as above (for $a(s)$ and $b(s)$) to conclude $A(s)=O(1)$ and $B(s)=O(\langle s\rangle^{-1-\mu})$, and the induction step is proved. Moreover, we have $A'(s)=O(\langle s\rangle^{-1-\mu})$, and the convergence of $\partial_x^\alpha\partial_\xi^\beta z^\lambda(t,x,\xi)=\partial_x^\alpha\partial_\xi^\beta a(t)$ is proved similarly.

Finally, we prove that $S_- : (x,\xi) \mapsto (z_-,\xi_-)$ is a local diffeomorphism. By the definition, we have

$$S_- \exp(TH_p) = S_-$$

for $T < 0$. If $|T|$ is sufficiently large, $\exp(TH_p)$ maps (x,ξ) to (x',ξ') such that $|x'| >> 0$ and $x'\cdot\xi' < -\delta|x'|\,|\xi'|$ with some $\delta > 0$. We show S_- is diffeomorphic in a neighborhood of (x',ξ') if $|x'|$ is sufficiently large.

We use the above argument for trajectory starting from (x',ξ'). Let $\varepsilon > 0$ be a small constant which we will specify later. Let $0 < \mu' < \mu$. If $|x'|$ is sufficiently large, then $A(s)$ and $B(s)$ above (with a new initial condition) satisfy

$$\begin{aligned} |A'(s)| &\le \varepsilon c_1 \langle s\rangle^{-1-\mu'}|A(s)| + c_1|B(s)| + \varepsilon c_1\langle s\rangle^{-1-\mu'}, \\ |B'(s)| &\le \varepsilon c_1 \langle s\rangle^{-2-\mu'}|A(s)| + \varepsilon c_1\langle s\rangle^{-1-\mu'}|B(s)| + \varepsilon c_1\langle s\rangle^{-2-\mu'} \end{aligned}$$

for $s \in [\lambda t_0, 0]$. Then, by carrying out the same argument as above, we learn $|A(t) - A(0)| \le c_2\varepsilon$. In particular, since $z^\lambda(0) = x + R\zeta^\lambda/|\zeta^\lambda|$, we have

$$|\partial_x(z^\lambda(t) - x)| \le c_3\varepsilon, \quad |\partial_\xi z^\lambda(t)| \le c_3,$$

where $t = \lambda t_0$. We recall, again by Proposition 2.10, we have

$$|\partial_x\eta^\lambda(t)| \le c_3\varepsilon, \quad |\partial_\xi(\eta^\lambda(t) - \xi)| \le c_3\varepsilon$$

if $|x'|$ is sufficiently large. Now if ε is sufficiently small (depending only on c_3),

$$(x',\xi') \mapsto (z^\lambda(t), \eta^\lambda(t))$$

has the Jacobian bounded from below by, for example, 1/2. We now fix $\varepsilon > 0$, and choose T (and hence (x',ξ')) accordingly. This Jacobian converges to that of S_- as $\lambda \to \infty$, and hence it is bounded from below by 1/2. Thus we learn that S_- is diffeomorphic in a neighborhood of (x',ξ') by the inverse function theorem. Since $\exp(TH_p)$ is diffeomorphic, this implies S_- is diffeomorphic in a neighborhood of (x,ξ). □

Note the above argument works for the scattering with $\exp tH_k$ also. In fact, the proof is simpler by virtue of the scaling property. For example, $(z^\lambda(s), \eta^\lambda(s))$ is independent of λ, the convergence follows immediately from the integrability of the derivative.

3 Proof of main theorems

3.1 Asymptotic motion and solutions to transport equations

We denote

$$\begin{aligned} z(t;x,\xi) &= y(t;x,\xi) - \partial_\xi W(t,\eta(t,x,\xi)), \\ z^\lambda(t;x,\xi) &= z(t/\lambda; x, \lambda\xi), \quad \eta^\lambda(t;x,\xi) = \eta(t/\lambda;x,\lambda\xi)/\lambda, \end{aligned}$$

and also

$$S_t : \ (x,\xi) \mapsto (z(t;x,\xi), \eta(t;x,\xi)),$$
$$S_t^\lambda : \ (x,\xi) \mapsto (z^\lambda(t;x,\xi), \eta^\lambda(t;x,\xi)).$$

S_t (resp. S_t^λ) is the Hamilton flow generated by

$$\ell(t;x,\xi) = p(x + \partial_\xi W(t,\xi), \xi) - \partial_t W(t,\xi)$$

($\ell^\lambda(t;x,\xi) = \lambda^{-2}\ell(t/\lambda, x, \lambda\xi)$, resp.) with the initial condition:

$$z(0,x,\xi) = x + R\xi/|\xi|, \quad \eta(0;x,\xi) = \xi$$

($z^\lambda(0,x,\xi) = x + R\xi/|\xi|$, $\eta^\lambda(0;x,\xi) = \xi$, resp.). By virtue of the Hamilton-Jacobi equation, we have

$$\ell(t,x,\xi) = p(x + \partial_\xi W(t,\xi), \xi) - p(\partial_\xi W(t,\xi), \xi)$$

for sufficiently large $|\xi|$.

Let $f_0(x,\xi)$ be a C_0^∞-function supported in a small neighborhood of $(x_0 + R\xi_0/|\xi_0|, \xi_0)$. We set

$$f_0^\lambda(x,\xi) = f_0(x, \xi/\lambda),$$

Then the solution to

$$\frac{\partial}{\partial t} f(t;\cdot,\cdot) = -\{\ell, f\}, \quad \text{with } \ f(0;x,\xi) = f_0^\lambda(x,\xi)$$

is given by

$$f(t;x,\xi) = f_0^\lambda \circ S_t^{-1}(x,\xi) \qquad \text{for } t \in [t_0, 0].$$

Similarly, the solution to

$$\frac{\partial}{\partial t} f^\lambda(t;\cdot,\cdot) = -\{\ell^\lambda, f^\lambda\}, \quad \text{with } \ f^\lambda(0;x,\xi) = f_0(x,\xi)$$

is given by

$$f^\lambda(t;x,\xi) = f_0 \circ (S_t^\lambda)^{-1}(x,\xi) \quad \text{for } t \in [\lambda t_0, 0].$$

It is easy to see $f^\lambda(t;x,\xi) = f(\lambda t; x, \xi/\lambda)$. By Proposition 2.12, we learn

$$S_-(x,\xi) = \lim_{\lambda\to+\infty} S_{\lambda t}^\lambda(x,\xi)$$

exists, and the all the derivatives converges locally uniformly (cf. the proof of Proposition 2.12). In particular, we have

$$\begin{aligned} f_-(x,\xi) &= \lim_{\lambda\to+\infty} f(t;x,\lambda\xi) = \lim_{\lambda\to+\infty} f^\lambda(\lambda t;x,\xi) \\ &= f_0 \circ (S_-)^{-1}(x,\xi) \in C_0^\infty(\mathbb{R}^{2n}) \end{aligned}$$

exists and it is independent of $t \in [t_0, 0)$. The convergence is locally uniform up to its derivatives.

3.2 Proof of Theorem 1.2

At first we consider

$$v(t) = e^{iW(t,D_x)}e^{-itH}v_0 \quad \text{for } t \in [t_0, 0]$$

with $v_0 \in L^2(\mathbb{R}^n)$. $v(t)$ satisfies the evolution equation:

$$\begin{aligned} \frac{d}{dt}v(t) &= e^{iW(t,D_x)}\Big\{ i\frac{\partial W}{\partial t}(t, D_x) - iH \Big\} e^{-itH}v_0 \\ &= -i\Big\{ e^{iW(t,D_x)}He^{-iW(t;D_x)} - \frac{\partial W}{\partial t}(t, D_x)\Big\} v(t). \end{aligned}$$

Namely, $v(t)$ is a solution to a Schrödinger equation with the time-dependent Hamiltonian:

$$L(t) = e^{iW(t,D_x)}He^{-iW(t,D_x)} - \frac{\partial W}{\partial t}(t, D_x).$$

The next lemma is basic in the following analysis.

Lemma 3.1. *Let $\nu, \rho > 0$ and suppose $a \in S\big(\langle x\rangle^\nu\langle\xi\rangle^\rho, dx^2/\langle x\rangle^2 + d\xi^2/\langle\xi\rangle^2\big)$. Let*

$$Q = e^{iW(t,D_x)}a(x, D_x)e^{-iW(t,D_x)}.$$

Then $Q \in OPS_K\big(\langle t\xi\rangle^\nu\langle\xi\rangle^\rho, dx^2/\langle t\xi\rangle^2 + d\xi^2/\langle\xi\rangle^2\big)$ with any $K \subset\subset \mathbb{R}^n$. Let $g(t; x, \xi) = \sigma(Q)$ be the Weyl symbol of Q. Then the principal symbol of Q is given by $a(x + \partial_\xi W(t, \xi), \xi)$ and

$$g(t; x, \xi) - a(x + \partial_\xi W(t, \xi), \xi) \in S_K\bigg(\langle t\xi\rangle^{\nu-2}\langle\xi\rangle^{\rho-2}, \frac{dx^2}{\langle t\xi\rangle^2} + \frac{d\xi^2}{\langle\xi\rangle^2}\bigg),$$

where the remainder is locally bounded in t with respect to the seminorms of the symbol class.

Proof. The proof is standard pseudodifferential operator calculus, but we sketch it for the completeness. Since the Weyl quantization has the same symbol representation in the Fourier space as in the configuration space, we may write

$$\hat{A}u := \mathcal{F}(a(x, D_x)\check{u}) = (2\pi)^{-n}\iint e^{-i(\xi-\eta)\cdot x}a(x, \tfrac{\xi+\eta}{2})u(\eta)\, d\eta\, dx$$

for $u \in \mathcal{S}(\mathbb{R}^n)$. By direct computations, we have

$$\begin{aligned} &e^{iW(t,\xi)}\hat{A}e^{-iW(t,\xi)}u(\xi) \\ &\quad = (2\pi)^{-n}\iint e^{i(W(t,\xi)-W(t,\eta))-i(\xi-\eta)\cdot x}a\big(x, \tfrac{\xi+\eta}{2}\big)u(\eta)\, d\eta\, dx \\ &\quad = (2\pi)^{-n}\iint e^{-i(\xi-\eta)\cdot(x-\tilde{W}(t,\xi,\eta))}a\big(x, \tfrac{\xi+\eta}{2}\big)u(\eta)\, d\eta\, dx \\ &\quad = (2\pi)^{-n}\iint e^{-i(\xi-\eta)\cdot x}a\big(x + \tilde{W}(t, \xi, \eta), \tfrac{\xi+\eta}{2}\big)u(\eta)\, d\eta\, dx, \end{aligned}$$

where

$$\tilde{W}(t,\xi,\eta)=\int_0^1 \partial_\xi W(t,s\xi+(1-s)\eta)\,ds.$$

We easily see

$$\left|\partial_\xi^\alpha\partial_\eta^\beta \tilde{W}(t,\xi,\eta)\right|\le C_{\alpha\beta}\langle\tfrac{\xi+\eta}{2}\rangle^{1-|\alpha-\beta|}\langle\xi-\eta\rangle^{1+|\alpha+\beta|},$$

for any $\alpha,\beta\in\mathbb{Z}_+^n$, and $\tilde{W}(t,\xi,\xi)=\partial_\xi W(t,\xi)$. Moreover, if $|\alpha|\ge 2$, by the definition of $W(t,\xi)$ and Proposition 2.10, we have

$$\left|\partial_\xi^\alpha W(t,\xi)\right|\le C_\alpha\big(\langle\xi\rangle^{1-|\alpha|}+|t|\langle\xi\rangle^{2-|\alpha|}\big), \tag{3.1}$$

and hence

$$\begin{aligned}
&\left|\partial_\xi^\alpha\partial_\eta^\beta \tilde{W}(t,\xi,\eta)\right|\\
&\quad\le C_{\alpha\beta}\bigg(\big\langle\tfrac{\xi+\eta}{2}\big\rangle^{-|\alpha+\beta|}\langle\xi-\eta\rangle^{|\alpha+\beta|}+|t|\big\langle\tfrac{\xi+\eta}{2}\big\rangle^{1-|\alpha+\beta|}\langle\xi-\eta\rangle^{1+|\alpha+\beta|}\bigg)\\
&\quad\le C_{\alpha\beta}\big\langle t\big(\tfrac{\xi+\eta}{2}\big)\big\rangle\big\langle\tfrac{\xi+\eta}{2}\big\rangle^{-|\alpha+\beta|}\langle\xi-\eta\rangle^{1+|\alpha+\beta|}.
\end{aligned}$$

We also note

$$\left|\tilde{W}(t,\xi,\eta)\right|\ge\delta\langle|t|\tfrac{\xi+\eta}{2}\rangle\quad\text{if }\xi\cdot\eta\ge\frac{1}{2}|\xi|\,|\eta|$$

with some $\delta>0$. Combining these, we can show

$$\begin{aligned}
&\left|\partial_x^\alpha\partial_\xi^\beta\partial_\eta^\gamma a(x+\tilde{W}(t,\xi,\eta),\tfrac{\xi+\eta}{2})\right|\\
&\quad\le C_{\alpha\beta\gamma}\langle t(\tfrac{\xi+\eta}{2})\rangle^{\nu-|\alpha|}\langle\tfrac{\xi+\eta}{2}\rangle^{\rho-|\beta+\gamma|}\langle\xi-\eta\rangle^{|\nu|+|\rho|+|\alpha+\beta+\gamma|}
\end{aligned}$$

for $x\in K\subset\subset\mathbb{R}^n$ and $\xi,\eta\in\mathbb{R}^n$. Then by the asymptotic expansion formula for the simplified symbol, we learn that the principal symbol is given by $a(x+\partial_\xi W(t,\xi),\xi)$. Moreover, we have

$$\left|\partial_x^\alpha\partial_\xi^\beta g(t;x,\xi)\right|\le C_{\alpha\beta}\langle t\xi\rangle^{\nu-|\alpha|}\langle\xi\rangle^{\rho-|\beta|}\quad\text{for }x\in K,\xi\in\mathbb{R}^n,$$

and the other claims follow from the asymptotic expansion formula. □

By Lemma 3.1, we learn that the principal symbol of $L(t)$ is given by $\ell(t;x,\xi)$, and the remainder symbol $r(t;x,\xi)$ satisfies

$$\left|\partial_x^\alpha\partial_\xi^\beta r(t;x,\xi)\right|\le C_{\alpha\beta}\big(\langle t\xi\rangle^{-\mu-2-|\alpha|}\langle\xi\rangle^{-|\beta|}+\langle t\xi\rangle^{-\mu-|\alpha|}\langle\xi\rangle^{-2-|\beta|}\big)$$

for $x\in K\subset\subset\mathbb{R}^n$, $t\in[t_0,0]$. Note that the subprincipal symbol vanishes by virtue of the Weyl calculus.

In order to prove Theorem 1.2, we characterize the wave front set of u_0 in terms of $u(t_0)=e^{-it_0H}u_0$ with $t_0<0$. Let $a\in C_0^\infty(\mathbb{R}^{2n})$ such that $a(x_0,\xi_0)\neq 0$ and supported in a small neighborhood of (x_0,ξ_0), and set

$$a^\lambda(x,\xi)=a(x,\xi/\lambda).$$

We also set

$$A^\lambda(t) = e^{iW(t,D_x)}e^{-itH}a^\lambda(x,D_x)e^{itH}e^{-iW(t,D_x)}$$

for $t \in [t_0, 0]$. A^λ satisfies the Heisenberg equation:

$$\frac{d}{dt}A^\lambda(t) = -i[L(t), A^\lambda(t)]. \tag{3.2}$$

We now construct an asymptotic solution of (3.1) with the initial condition:

$$A^\lambda(0) = e^{iW(0,D_x)}a^\lambda(x,D_x)e^{-iW(0,D_x)} = \tilde{a}^\lambda(x,D_x).$$

We note that the principal symbol of $\tilde{a}^\lambda(x,\xi)$ is give by $a(x - R\hat{\xi}, \xi/\lambda)$, and $\tilde{a}^\lambda(x,\xi)$ is supported in a neighborhood of $(x_0 + R\hat{\xi}_0, \lambda\xi_0)$ modulo $O(\lambda^{-\infty})$-terms, where we denote $\hat{\xi} = \xi/|\xi|$.

We note that if $A^\lambda(t)$ is a pseudodifferential operator, the principal symbol of the right hand side of (3.2) is given by $-\{\ell, a^\lambda\}$, where $a^\lambda(t;\cdot,\cdot)$ is the symbol of $A^\lambda(t)$. Then by the computation in Subsection 3.1, we learn that $a^\lambda \circ S_t^{-1}$ is an approximate solution to the transport equation. Actually, we can construct an asymptotic solution to (3.2):

Proposition 3.2. *Let $a \in C_0^\infty(\mathbb{R}^{2n})$ supported in a sufficiently small neighborhood of (x_0, ξ_0). Then there exists $\psi^\lambda(t;\cdot,\cdot) \in C_0^\infty(\mathbb{R}^{2n})$ such that*

(i) *We write $G^\lambda(t) = \psi^\lambda(t; x, D_x)$. Then*

$$G^\lambda(0) = e^{iW(0,D_x)}a^\lambda(x,D_x)e^{-iW(0,D_x)}$$

modulo $O(\lambda^{-\infty})$-terms.

(ii) *$\psi^\lambda(t;\cdot,\cdot)$ is supported in $S_t[\mathrm{supp}\, a^\lambda]$.*

(iii) *For any $\alpha, \beta \in \mathbb{Z}_+^n$, there is $C_{\alpha\beta} > 0$ such that*

$$\left|\partial_x^\alpha \partial_\xi^\beta \psi^\lambda(t; x, \xi)\right| \le C_{\alpha\beta}\lambda^{-|\beta|}, \quad t \in [t_0, 0],\ x, \xi \in \mathbb{R}^n,\ \lambda \gg 0.$$

(iv) *The principal symbol of ψ^λ is given by $a^\lambda \circ S_t^{-1}$, i.e.,*

$$\left|\partial_x^\alpha \partial_\xi^\beta \left(\psi^\lambda(t;x,\xi) - a^\lambda \circ S_t^{-1}(x,\xi)\right)\right| \le C_{\alpha\beta}\lambda^{-1-|\beta|}$$

for $t \in [t_0, 0]$, $x, \xi \in \mathbb{R}^n$, $\lambda \gg 0$.

(v) *For $t \in [t_0, 0]$,*

$$\left\|\frac{d}{dt}G^\lambda(t) + i[L(t), G^\lambda(t)]\right\|_{\mathcal{L}(L^2(\mathbb{R}^n))} = O(\lambda^{-\infty}) \quad \textit{as } \lambda \to +\infty.$$

We postpone the proof of Proposition 3.2 to the next subsection, and we complete the proof of Theorem 1.2.

Proof of Theorem 1.2. By Proposition 3.2 and the construction of $L(t)$, we have

$$\left\| \frac{d}{dt}\Big(e^{itH} e^{-iW(t,D_x)} G^\lambda(t) e^{iW(t,D_x)} e^{-itH} \Big) \right\| \le C_N \lambda^{-N}$$

with any N as $\lambda \to +\infty$. This implies

$$\Big\| e^{it_0 H} e^{-iW(t_0,D_x)} G^\lambda(t_0) e^{iW(t_0,D_x)} e^{-it_0 H} u_0 \\ - e^{-iW(0,D_x)} G^\lambda(0) e^{iW(0,D_x)} u_0 \Big\| \le C_N \lambda^{-N}.$$

By the condition (i) of Proposition 3.2, we have

$$\Big| \big\| G^\lambda(t_0) e^{iW(t_0,D_x)} u(t_0) \big\| - \big\| a^\lambda(x,D_x) u_0 \big\| \Big| \le C_N \lambda^{-N}, \tag{3.3}$$

where $u(t) = e^{-itH} u_0$. We note that $\psi^\lambda(t_0; x,\xi)$ is supported in $S_{t_0}[\mathrm{supp}\, a^\lambda]$, and the principal symbol is given by $a^\lambda \circ S_{t_0}^{-1}$. Hence, in particular,

$$|\psi^\lambda(t_0; x, \xi)| \ge \varepsilon > 0 \tag{3.4}$$

for $|x - z_-(x_0,\xi_0)| \le \delta$, $|\xi - \lambda\xi_-(x_0,\xi_0)| \le \delta\lambda$ and $\lambda \gg 0$ with some $\delta, \varepsilon > 0$.

Now we suppose $(x_0,\xi_0) \notin WF(u_0)$. Then by choosing a supported in a sufficiently small neighborhood of (x_0,ξ_0), we may suppose

$$\|a^\lambda(x,D_x)u_0\| = O(\lambda^{-\infty}) \quad \text{as } \lambda \to +\infty.$$

Then by (3.3) we have

$$\big\| G^\lambda(t_0) e^{iW(t_0,D_x)} u(t_0) \big\| = O(\lambda^{-\infty}) \tag{3.5}$$

and this implies

$$(z_-(x_0,\xi_0), \xi_-(x_0,\xi_0)) \notin WF\big(e^{iW(t_0,D_x)} u(t_0) \big)$$

by virtue of (3.4).

Conversely, if $(z_-(x_0,\xi_0), \xi_0(x_0,\xi_0)) \notin WF(e^{iW(t_0,D_x)}u(t_0))$ then also by taking a supported in a sufficiently small neighborhood of (x_0,ξ_0), we have (3.5) since $\psi^\lambda(t_0;\cdot,\cdot)$ is supported in $S_{t_0}[\mathrm{supp}\, a^\lambda]$ modulo $O(\lambda^{-\infty})$-terms, and it is very close to $S_-[\mathrm{supp}\, a^\lambda]$ if λ is large. Then again by (3.3), we have $\|a^\lambda(x,D_x)u_0\| = O(\lambda^{-\infty})$, and hence $(x_0,\xi_0) \notin WF(u_0)$. $\square$

3.3 Proof of Proposition 3.2

We note
$$R+\delta|t\xi|\le|\partial_\xi W(t,\xi)|\le R+C|t\xi|$$
for $t\in[t_0,0]$, $\xi\in\mathbb{R}^n$ with some $\delta,C>0$. Using this and (3.1), for any $\alpha,\beta\in\mathbb{Z}_+^n$ and $K\subset\subset\mathbb{R}^n$, we have
$$\left|\partial_x^\alpha\partial_\xi^\beta\ell(t;x,\xi)\right|\le C_{\alpha\beta K}\big(\langle t\xi\rangle^{-1-\mu-|\alpha|}\langle\xi\rangle^{2-|\beta|}+\langle t\xi\rangle^{1-\mu-|\alpha|}\langle\xi\rangle^{-|\beta|}\big)$$
for $t\in[t_0,0]$, $x\in K$ and $\xi\in\mathbb{R}^n$.

Let $a_0^\lambda\in C_0^\infty(\mathbb{R}^{2n})$ such that
$$e^{iW(0,D_x)}a^\lambda(x,D_x)e^{-iW(0,D_x)}=(a_0^\lambda\circ S_0^{-1})(x,D_x)$$
modulo $O(\lambda^{-\infty})$-terms. It is easy to see that the principal symbol of a_0^λ is $a^\lambda(x,\xi)$, and that $a_0^\lambda\in S(1,dx^2+\lambda^{-2}d\xi^2)$. We may suppose supp $a_0^\lambda=$ supp a^λ. We now set
$$\psi_0(t;x,\xi)=a_0^\lambda\circ S_t^{-1}(x,\xi).$$
Then as we observed in Subsection 3.1, ψ^λ satisfies
$$\frac{\partial}{\partial t}\psi_0(t;x,\xi)=-\{\ell,\psi_0\}(t;x,\xi).$$
We set
$$r_0(t;x,\xi)=\frac{\partial}{\partial t}\psi_0(t;x,D_x)+i[L(t),\psi_0(t;x,D_x)].$$
Then by the asymptotic expansion formula, $r_0\in S(\lambda^{-1},dx^2+\lambda^{-2}d\xi^2)$, and r_0 is supported essentially (i.e., modulo $O(\lambda^{-\infty})$-terms) in $S_t[\text{supp } a^\lambda]$. Next we solve the transport equation:
$$\frac{\partial}{\partial t}\psi_1(t;x,\xi)+\{\ell,\psi_1\}(t;x,\xi)=-r_0(t;x,\xi)$$
with the initial condition $\psi_1(0;x,\xi)=0$. It is easy to show that $\psi_1(t,\cdot,\cdot)\in S(\lambda^{-1},dx^2+\lambda^{-2}d\xi^2)$ and it is bounded in $t\in[t_0,0]$. Moreover, ψ_1 is supported in $S_t[\text{supp } a^\lambda]$.

We set
$$r_1(t;x,\xi)=\frac{\partial}{\partial t}\psi_1(t;x,\xi)+i[L(t),\psi_1(t;x,D_x)]+r_0(t;x,D_x),$$
then $r_1(t;\cdot,\cdot)\in S(\lambda^{-2},dx^2+\lambda^{-2}d\xi^2)$ and supp $r_1(t;\cdot,\cdot)\subset S_t[\text{supp } a^\lambda]$ essentially for $t\in[t_0,0]$. We iterate this procedure to obtain $\psi_j\in S(\lambda^{-j},dx^2+\lambda^{-2}d\xi^2)$ such that supp $\psi_j(t;\cdot,\cdot)\subset S_t[\text{supp } a^\lambda]$ essentially for $t\in[t_0,0]$. Then we set
$$\psi^\lambda(t;x,\xi)\sim\sum_{j=0}^\infty\psi_j(t;x,\xi)\in S(1,dx^2+\lambda^{-2}d\xi^2)$$

in the sense of the asymptotic sum as $\lambda \to +\infty$. By the construction of the asymptotic sum, we may suppose $\operatorname{supp} \psi^\lambda(t;\cdot,\cdot) \subset S_t[\operatorname{supp} a^\lambda]$ essentially for $t \in [t_0, 0]$. Now it is straightforward to check ψ satisfies the required properties. $\square$

3.4 Proof of Theorem 1.1

We denote

$$T_t(x,\xi) = (x - \partial_\xi W(t,\xi), \xi)$$

so that

$$S_t = T_t \circ \exp tH_p.$$

We also denote

$$b_t^\lambda(x,\xi) = a^\lambda \circ \exp(-tH_p)(x,\xi).$$

Then, in order to prove Theorem 1.1, it suffices to show

$$\left\| b_{t_0}^\lambda(x, D_x) u(t_0) \right\| = O(\lambda^{-\infty}) \quad \text{as } \lambda \to +\infty$$

if and only if $(x_0, \xi_0) \notin WF(u_0)$, where $u(t) = e^{-itH} u_0$, a is supported in a small neighborhood of (x_0, ξ_0) and $t_0 < 0$. We note

$$b_t^\lambda = a^\lambda \circ [\exp tH_p]^{-1} = a^\lambda \circ S_t^{-1} \circ T_t,$$

namely,

$$b_t^\lambda(x,\xi) = (a^\lambda \circ S_t^{-1})(x - \partial_\xi W(t,\xi), \xi).$$

By direct computations as in the proof of Lemma 3.1, we can show

$$e^{iW(t,D_x)} b_t^\lambda(x, D_x) e^{-iW(t,D_x)} = c_t^\lambda(x, D_x)$$

where $c_t^\lambda \in C_0^\infty(\mathbb{R}^n)$ modulo $O(\lambda^{-\infty})$, and as an h-pseudodifferential operator (with $h = \lambda^{-1}$), the principal symbol is given by $(a^\lambda \circ S_t^{-1})(x,\xi) = (a \circ (S_{\lambda t}^\lambda)^{-1})(x, \xi/\lambda)$. Moreover, if we write $\tilde{c}_t^\lambda(x,\xi) = c_t^\lambda(x, \lambda\xi)$, then $\tilde{c}_t^\lambda$ is supported in an arbitrarily small neighborhood of $S_-[\operatorname{supp} a]$ if λ is sufficiently large, and the principal symbol is $a \circ (S_{\lambda t}^\lambda)^{-1}$. We can also show (as in Lemma 3.1) that $\tilde{c}_t^\lambda$ is bounded in $C_0^\infty(\mathbb{R}^{2n})$ as $\lambda \to \infty$. Since

$$\left\| b_{t_0}^\lambda(x, D_x) u(t_0) \right\| = \left\| \tilde{c}_t^\lambda(x, hD_x) e^{iW(t,D_x)} u(t_0) \right\|,$$

now Theorem 1.1 follows from Theorem 1.2 combined with the standard characterization of the wave front set in terms of h-pseudodifferential operators. $\square$

A Appendix

Lemma A.1. *Suppose $n \geq 2$, $f \in C^1(\mathbb{R}^n)$ and suppose*

$$\left|\partial_x f(x)\right| \leq C\langle x\rangle^\beta, \quad x \in \mathbb{R}^n,$$

with some $C > 0$, $\beta \in \mathbb{R}$. Then

$$\left|f(x) - f(y)\right| \leq (\pi/2)C \max(\langle x\rangle^\beta, \langle y\rangle^\beta)|x - y|.$$

The same estimate holds for $n = 1$ if $x \cdot y > 0$.

Proof. The claim is obvious if $\beta \geq 0$ or $n = 1$, and we suppose $n \geq 2$ and $\beta < 0$. Let $|x| \geq |y| \geq 0$ and let $S = \left\{z \in \mathbb{R}^n \;\middle|\; |z| = |y|\right\}$ be the sphere of radius $|y|$ with the center at the origin. Let ℓ be the (straight) line segment connecting x and y. If ℓ and S intersect only at y, then we can use the standard argument of show

$$|f(x) - f(y)| = \int_\ell |\nabla f(z)|\,|dz| \leq C\langle y\rangle^\beta |x - y|.$$

If ℓ and S intersect at y and y', we denote the line segments connecting y and y', and y' and x, by ℓ' and ℓ'', respectively. Then $|x-y| = |\ell| = |\ell'|+|\ell''|$. We note the length of the shortest geodesic connecting y and y' on S (which we denote by γ_1) is equal to or less than $(\pi/2)|\ell'|$. We set $\gamma = \gamma_1 + \ell''$, which is a piecewise C^1-path connecting y and x, and

$$|\gamma| \leq (\pi/2)|\ell'| + |\ell''| \leq (\pi/2)|x - y|.$$

Since γ is contained in $\{z \,|\, |z| \geq |y|\}$, we have

$$|f(x) - f(y)| \leq \int_\gamma |\nabla f(z)|\,|dz| \leq C\langle y\rangle^\beta (\pi/2)|x - y|.$$

□

References

[1] Bouclet, J.-M., Tzvetkov, N.: Strichartz estimates for long range perturbations. Preprint, 2005 Sep.

[2] Boutet de Monvel, L.: Propagation des singularités des solutions d'equation de Schrödinger, *in* Fourier Integral Operators and Partial Differential Equations, Springer L. N. M. **459**, 1975.

[3] Burq, N., Gérard, P., Tzvetkov, N.: Strichartz inequalities and the nonlinear Schrödinger equation on compact manifolds, American J. Math. **126**, 569–605 (2004).

[4] Craig, W., Kappeler, T., Strauss, W.: Microlocal disipertive smoothing for the Schrödinger equation. Comm. Pure Appl. Math. **48**, 769–860 (1996).

[5] Dimassi, M., Sjöstrand, J.: *Spectral Asymptotics in the Semi-Classical Limit*. London Math. Soc. Lecture Notes Series **268**, 1999.

[6] Doi, S.: Singularities of solutions of Schrödinger equations for perturbed harmonic oscillators. Hyperbolic problems and related topics, 185–199, Grad. Ser. Anal., Int. Press, Somerville, MA, 2003.

[7] Doi, S.: Smoothness of solutions for Schrödinger equations with unbounded potentials. Publ. Res. Inst. Math. Sci. **41**, 175–221 (2005).

[8] Hassel, A., Wunsch, J.: The Schrödinger propagator for scattering metrics. Ann. Math. **162**, 487–523 (2005).

[9] Hörmander, L.: The existence of wave operators in scattering theory. Math. Zeitschrift **146**, 69–91 (1976).

[10] Hörmander, L.: *Analysis of Linear Partial Differential Operators*, Vol. I-IV. Springer Verlag, 1983–1985.

[11] Ito, K.: Propagation of singularities for Schrödinger equations on the Euclidean space with a scattering metric. Comm. Partial Differential Equations **31**, 1735–1777 (2006).

[12] Kapitanski, L., Rodnianski, I. and Yajima, K.: On the fundamental solution of a perturbed harmonic oscillator, Topol. Methods Nonlinear Anal. **9**, 77–106 (1997).

[13] Lascar, R.: Propagation des singularités des solutions d'équations pseudo-differentialles quasi-homogenes. Ann. Inst. Fourier (Grenoble) **27**, 79–123 (1977).

[14] Martinez, A.: *An Introduction to Semiclassical and Microlocal Analysis*, Universitext, Springer Verlag New York 2002.

[15] Martinez, A., Nakamura, S., Sordoni, V.: Analytic Smoothing Effect for the Schrödinger Equation with Long-Range Perturbation, Comm. Pure Appl. Math. **59**, 1330–1351 (2006).

[16] Nakamura, S.: Propagation of the homogeneous wave front set for Schrödinger equations. Duke Math. J. **126**, 349-367 (2005)

[17] Nakamura, S.: Wave front set for solutions to Schrödinger equations. Preprint 2004.

[18] Reed, M., Simon, B.: *The Methods of Modern Mathematical Physics*, Vol. I–IV. Academic Press, 1972–1980.

[19] Robbiano, L., Zuily, C.: Microlocal analytic smoothing effect for the Schrödinger equation, Duke Math. J., **100** (1999), 93–129.

[20] Robbiano, L., Zuily, C.: Analytic Theory for the Quadratic Scattering Wave Front Set and Application to the Schrödinger Equation. Soc. Math. France, Astérisque **283** (2002), 1–128.

[21] Robbiano, L., Zuily, C.: Strichartz estimates for Schrödinger equations with variable coefficients. Mém. Soc. Math. Fr. (N.S.) **101-102**, 1–208 (2005).

[22] Staffilani, G., Tataru, D.: Strichartz estimates for a Schrödinger operator with non smooth coefficients. Com. P. D. E. **27**, 1337–1372 (2002).

[23] Wunsch, J.: Propagation of singularities and growth for Schrödinger operators. Duke Math. J. **98**, 137–186 (1999).

[24] Yajima, K.: Smoothness and non-smoothness of the fundamental solution of time dependent Schrödinger equations. Comm. Math. Phys. **181**, 605–629 (1996).

[25] Yamazaki, M.: On the microlocal smoothing effect of dispersive partial differential equations I: second order linear equations. *Algebraic Analysis* Vol. II, 911–926, Academic Press, 1988.

[26] Zelditch, S.: Reconstruction of singularities for solutions of Schrödinger's equation. Commun. Math. Phys. **90**, 1–26 (1983).